Concurrent multi-scale modelling of vacuum arc plasma initiation

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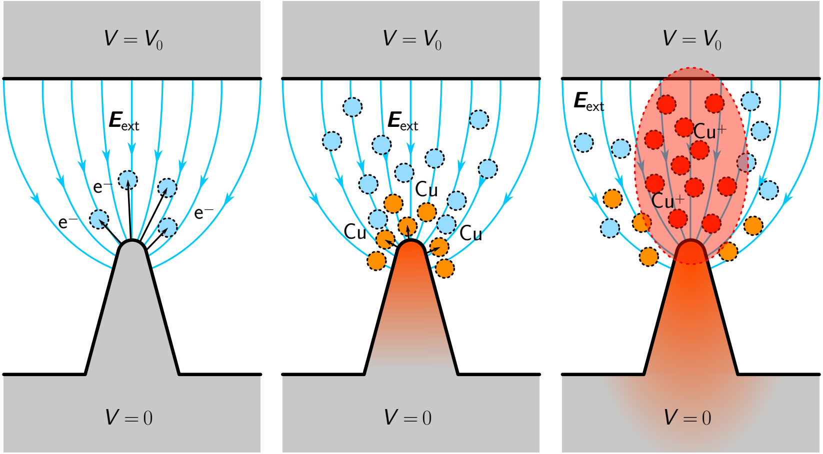
Outline

1. Vacuum arc background
2. Simulation methods
    - Field solution using finite element method (FEM)
    - Particle-in-cell (PIC) simulation of plasma
    - Binary collisions
3. Simulation model additions
    - Dynamic weighting
    - Field ionization
    - Ion bombardment
    - Circuit model
4. Static nanotip simulation
5. Conclusions

Stages of vacuum arc plasma formation



Stage 1: field emission Stage 2: heating and evaporation Stage 3: ionization

Figure 1: Initial stages of plasma formation.

Electric field, emission, heating

- Assume field emitter on surface → field enhancement → field emission of electrons
- Two main heating effects: Nottingham heating on the surface and Joule (resistive) heating in the bulk
- Evaporation of neutrals causes cooling
- Particle bombardment deposits additional heat on surface as plasma starts forming

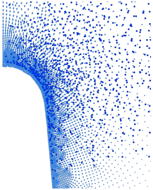


Figure 2: Field and electrons.

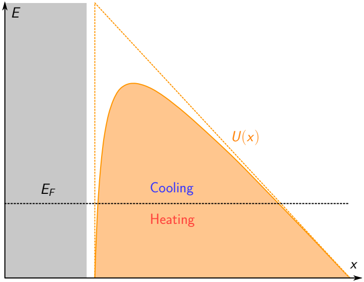


Figure 3: Electron $\langle \Delta E \rangle$ → cooling/heating. Figure adapted from [1].

[1] A. Kyritsakis. Electron emission calculations beyond the classical equations: finite size, space charge and thermal effects in sharp emitters. IVNC 2021.

Vacuum arc simulations

- Previous ArcPIC [2] code focused on plasma simulation, no heating effects
- FEMOCS (Finite Elements on Crystal Surfaces) code [3]
  - Concurrent, multi-scale, multi-physics
  - Finite element method (FEM), particle-in-cell method (PIC), connects to molecular dynamics (MD)
  - Combines electric field and heating calculations
  - Emission calculated using GETELEC code
- Current work: Simulation of initial plasma around static nanotip

[2] H. Timko et al. From field emission to vacuum arc ignition: A new tool for simulating copper vacuum arcs. Contributions to Plasma Physics, 2015.

[3] M. Veske et al. Dynamic coupling between particle-in-cell and atomistic simulations. Phys. Rev E., 2020.

Field solution using finite element method (FEM)

- Solve PDEs of system using finite element method
- Poisson's equation
  $\nabla \cdot (\varepsilon_0 \nabla \phi) = -\rho$ in vacuum
  $\rightarrow$ electric field
- Continuity equation
  $\nabla \cdot (\sigma \nabla \phi) = 0$ in bulk
  $\rightarrow$ current density
- Heat equation
  $\nabla \cdot (\kappa \nabla T) + P_J = C_v \partial_t T$ in bulk
  $\rightarrow$ temperature

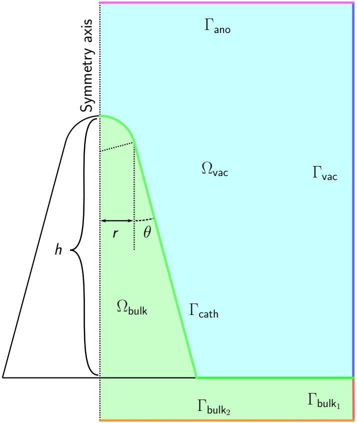


Figure 4: Domains in simulation, vacuum (blue) and bulk Cu (green).

Particle-in-cell (PIC) simulation of plasma

- Particles injected to system at cathode surface (emitted electrons, evaporated neutrals)
- Large number of particles e.g. electrons can be modelled as super-particles (SPs)

1. Calculate motion of particles in cell (e.g. leapfrog method)
2. Calculate electric field for mesh (solve Poisson's equation using FEM)
3. Do Monte Carlo collisions between particles within each cell

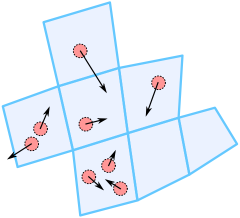


Figure 5: SPs in mesh.

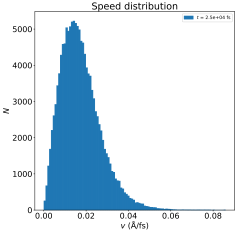


Figure 6: Speed distribution of neutrals.

Binary collisions

- Particles within a cell are matched randomly in pairs
- All interactions approximated by simple two-body processes [5]

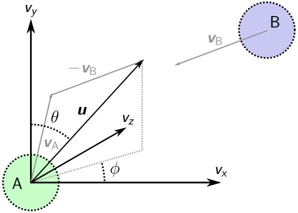


Figure 7: Coordinate system.

Velocity calculation for elastic collision of particles A and B [4]

$$\Delta \boldsymbol{u} = R^{-1}(\theta,\phi)\left(R^{-1}(\Theta,\Phi) - I\right)(0,0,u)^\mathrm{T}, \tag{1}$$

$$\boldsymbol{v}_A' = \boldsymbol{v}_A + \mu/m_A \Delta\boldsymbol{u}, \tag{2}$$

$$\boldsymbol{v}_B' = \boldsymbol{v}_B - \mu/m_B \Delta\boldsymbol{u}, \tag{3}$$

where $\mu = \frac{m_A m_B}{m_A + m_B}$ is the effective mass, u is relative velocity and R is a rotation matrix with angles $\Phi \sim U(0, 2\pi)$ and $\cos\Theta \sim U(-1, 1)$.

[4] T. Takizuka and H. Abe. A binary collision model for plasma simulation with a particle code. Journal of Computational Physics, 1977.

Collision types

1. Elastic collisions
    1. $\mathrm{Cu} + \mathrm{e}^- \rightarrow \mathrm{Cu} + \mathrm{e}^-$
    2. $\mathrm{Cu} + \mathrm{Cu} \rightarrow \mathrm{Cu} + \mathrm{Cu}$
2. Coulomb collisions for all charged particles
3. Impact ionization
    1. Neutrals: $\mathrm{Cu} + \mathrm{e}^- \rightarrow \mathrm{Cu}^{n+} + (\mathrm{n} + 1)\ \mathrm{e}^-$
    2. Ions: $\mathrm{Cu}^{i+} + \mathrm{e}^- \rightarrow \mathrm{Cu}^{(i+n)+} + (\mathrm{n} + 1)\ \mathrm{e}^-$
4. Charge exchange: $\mathrm{Cu} + \mathrm{Cu}^+ \rightarrow \mathrm{Cu}^+ + \mathrm{Cu}$
5. Radiative recombination: $\mathrm{Cu}^+ + \mathrm{e}^- \rightarrow \mathrm{Cu} + (\gamma)$

Collision probability [5]

Collision takes place when $R \sim U(0,1) < P$,

$$P = 1 - \exp\left(-un\sigma(E)\Delta t\right), \quad (4)$$

where n is the lower density of the two colliding particle types, σ is the cross section and Δt is time step.

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[5] V. Vahedi and M. Surendra. A Monte Carlo collision model for the particle-in-cell method: applications to argon and oxygen discharges. Computer Physics Communications, 1995.

Dynamic weighting

- Particle weights can be changed during their lifetime
- This means that particles can react even though their weights are not the same
- Reacting an electron of weight 20 with a neutral of weight 1 would leave behind an electron of weight 19, this requires splitting the SPs
- We can also make particle weights larger by merging SPs to speed up simulations

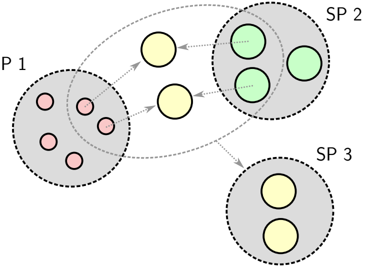


Figure 8: Splitting.

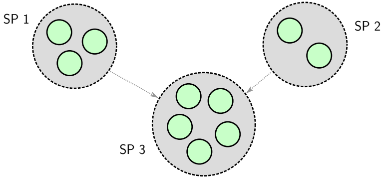


Figure 9: Merging.

Field ionization

- Evaporated neutrals ionized directly by tunneling [6]
- Expected to dominate ionization processes when field is high
- Ammosov–Delone–Krainov (ADK) model

Probability of direct field ionization [7]

$$P = 1.52 \times \frac{4^n \xi}{n\, \Gamma(2n)} \left(20.5 \frac{\xi^{3/2}}{E}\right)^{2n-1} \exp\left(-6.83 \frac{\xi^{3/2}}{E}\right), \tag{5}$$

where $n = 3.69 z \xi^{-1/2}$ and P is probability (1 / fs), ξ is the potential of ionization (eV), E is the electric field (GV / m) and z is charge after ionization.

[6] D. Bruhwiler et al. Particle-in-cell simulations of tunneling ionization effects in plasma-based accelerators. Physics of Plasmas, 2003.

[7] S. Calatroni. Direct field ionization. In 8th International Workshop on Mechanisms of Vacuum Arcs, 2019.

Ion bombardment

- Ions are accelerated by the electric field
- Two effects: sputtering and bombardment heating
- Ions can cause neutrals to be sputtered from the surface depending on energy → sputtering yield
- Remaining energy is deposited as heat into the surface

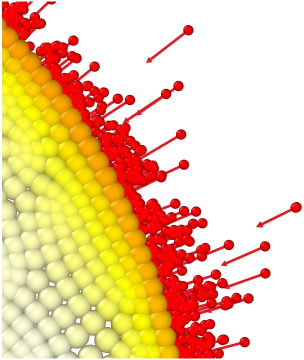


Figure 10: Cu^{+} ions (red) bombarding cathode surface.

Circuit model

- In real circuits we always have resistance, capacitance and inductance
- Added circuit model with resistor $I_{\mathrm{circ}} = \frac{U - V_{\mathrm{gap}}}{R}$ and capacitor
- Gap forms a capacitor with $C_{\mathrm{gap}} = Q_{\mathrm{gap}} / V_{\mathrm{gap}}$ and $I_{\mathrm{cap}} = I_{\mathrm{gap}} - I_{\mathrm{circ}}$
- Calculate gap current I_{gap} from Shockley-Ramo theorem

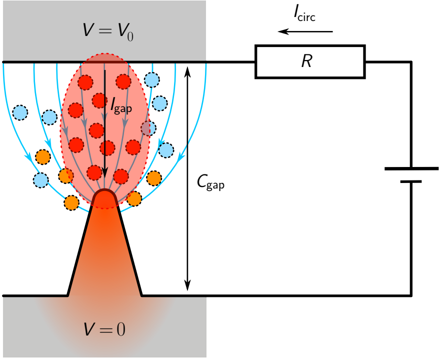


Figure 11: Vacuum arc circuit.

Present simulation model

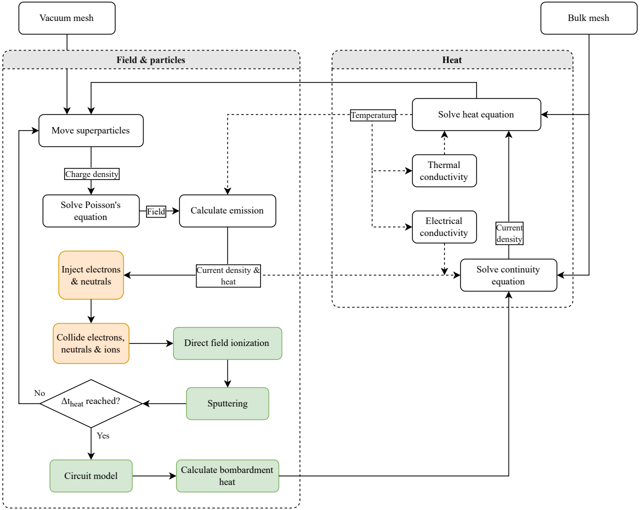


Figure 12: Flowchart of present model with PIC additions, excluding MD.

Heating of static nanotip

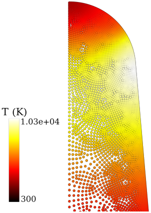


Figure 13: Tip with $\theta = 5^\circ$, JH.

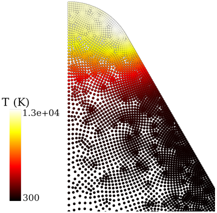


Figure 15: Tip with $\theta = 30^\circ$, JH.

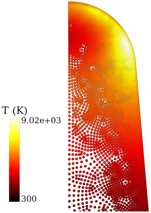


Figure 14: Tip with $\theta = 5^\circ$, JH+NH.

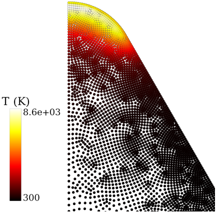


Figure 16: Tip with $\theta = 30^\circ$, JH+NH.

Simulation 1

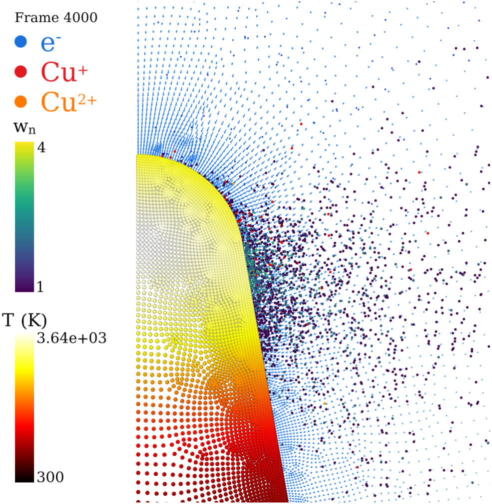


Figure 17: Nanotip $r = 50$ nm, $h = 10r$, $V_0 = 1$ kV, $E_{\mathrm{loc}} = 10.8$ GV/m.

Simulation 2

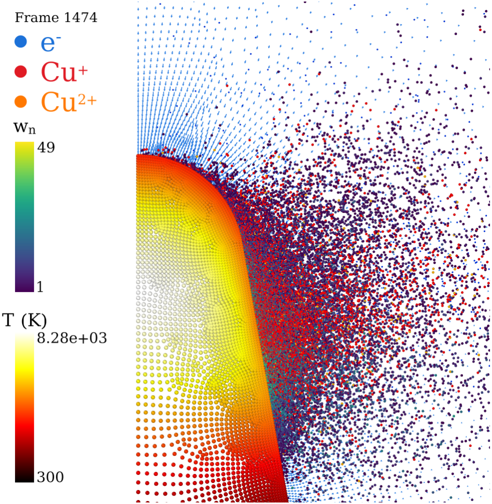
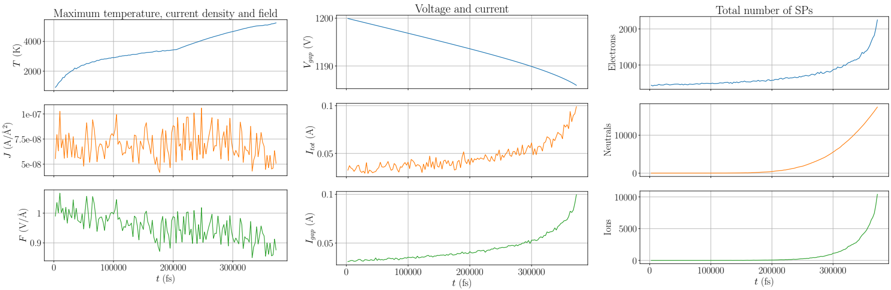


Figure 18: Nanotip $r = 50$ nm, $h = 10r$, $V_0 = 1.2$ kV.

Simulation 2

- What are the thresholds for thermal runaway?



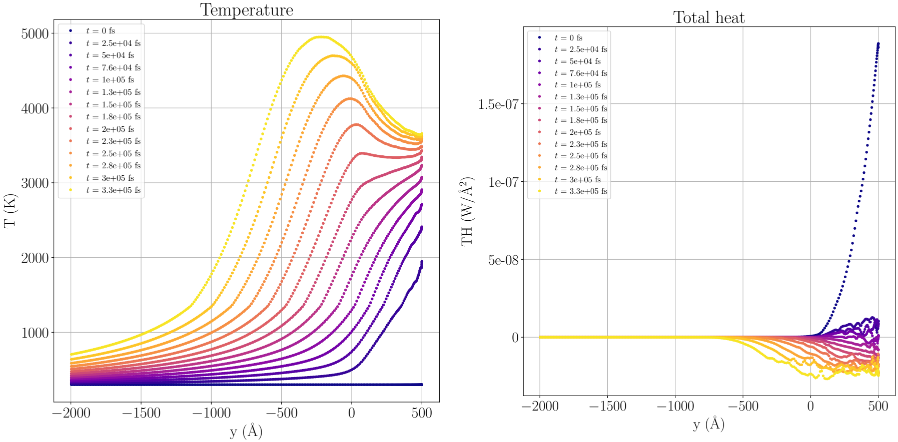
(a) Temperature, current density and field.

(b) Voltage and total/gap current.

(c) Number of superparticles.

Figure 19: System state for 50 nm tip, ECI collisions.

Simulation 2



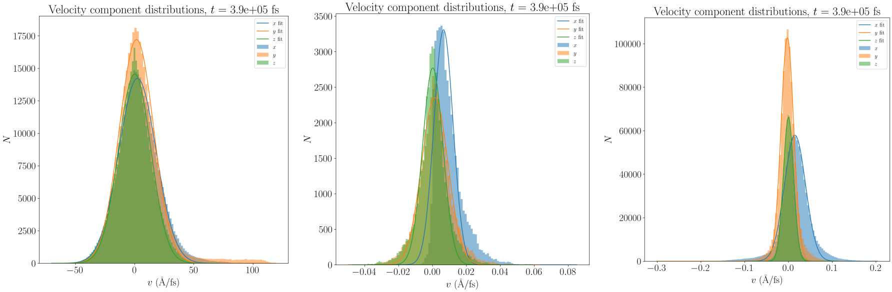
(a) Temperature of cathode surface.

(b) Total heat on cathode surface.

Figure 20: Nanotip heating.

Simulation 2

- Velocities of particles show expansion of plasma, fitted Gaussians indicate MB distribution

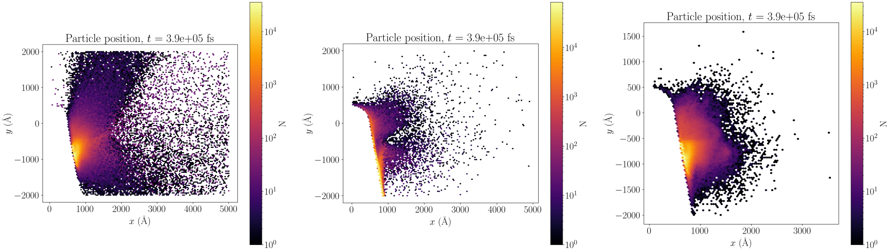


(a) Electrons. (b) Neutrals. (c) Ions.

Figure 21: Velocity component distributions of particles.

Simulation 2

- Electron and neutral distributions show how ions formed

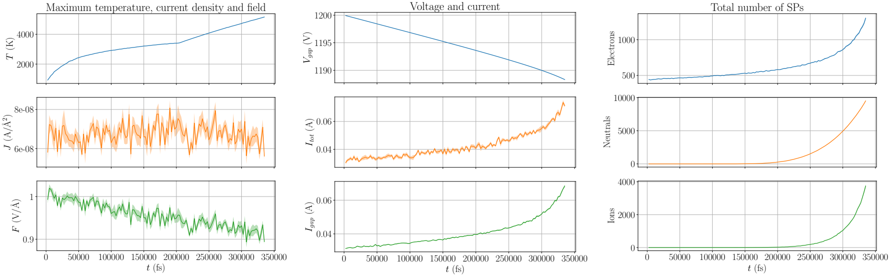


(a) Electrons. (b) Neutrals. (c) Ions.

Figure 22: Positions of particles.

Simulation 3

- What interactions are most significant for runaway?



(a) Temperature, current density and field.

(b) Voltage and total/gap current.

(c) Number of superparticles.

Figure 23: Mean system state (8 runs) for 50 nm tip, 1.2 kV, ECIFBS[1].

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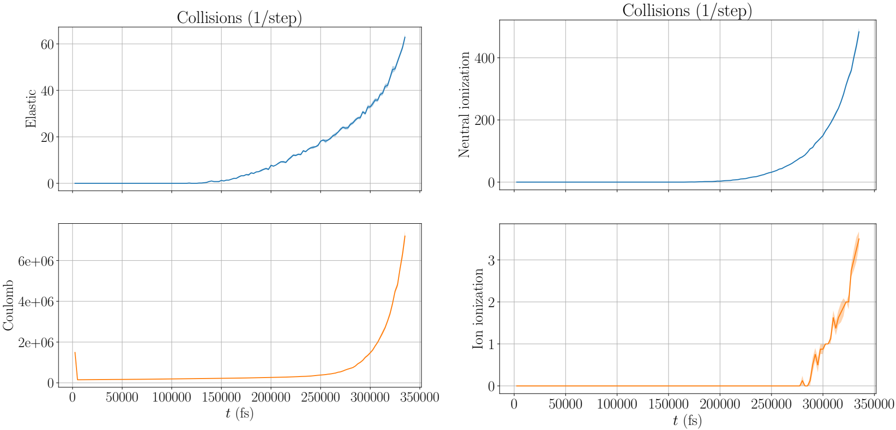
[1] elastic, Coulomb, ionization, field ionization, bombardment heating, sputtering

Simulation 3



(a) Elastic collisions.

(b) Neutral and ion ionizations.

Figure 24: Number of collisions per timestep.

Simulation 3

- Out of all ionizations, over 10% are field ionizations
- Few sputtered neutrals, bombardment mostly heat

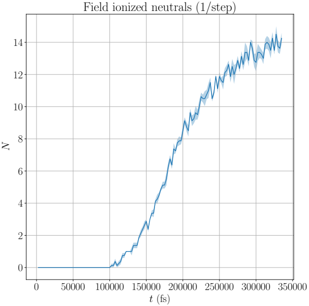


Figure 25: Number of field ionizations per timestep.

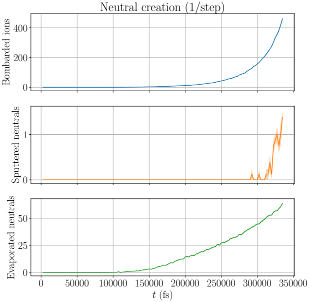


Figure 26: Neutral creation processes.

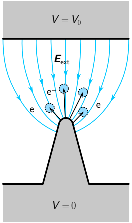
Conclusions

- Accurate simulation of plasmas relies on accurate modelling of particle interactions such as collisions
- Runaway is possible with these interactions on their own!
- Runaway threshold of approximately 10 GV/m roughly agrees with experiments
- Field ionization significant at fields on the order of 10 GV/m, sputtering less significant for initial formation of plasma
- Future work: molecular dynamics

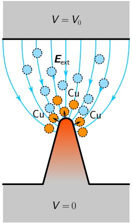
Thanks to everyone working on the project!

Special thanks:
Andreas Kyritsakis Flyura Djurabekova
Mihkel Veske Tauno Tiirats

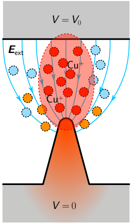
Thank you! Questions, comments?



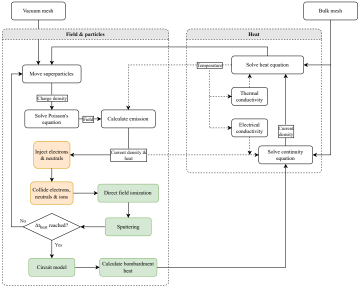
Stage 1: field emission



Stage 2: heating and evaporation



Stage 3: ionization



Vacuum mesh

Bulk mesh

Field & particles

Move superparticles

Charge density

Solve Poisson's equation

Field

Calculate emission

Current density & heat

Inject electrons & neutrals

Collide electrons, neutrals & ions

Direct field ionization

Sputtering

Δt_{heat} reached?

No

Yes

Circuit model

Calculate bombardment heat

Heat

Solve heat equation

Temperature

Thermal conductivity

Electrical conductivity

Current density

Solve continuity equation